

Pentyl 2-hydroxypropanoate
6382-06-5 | DTXSID70858752

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.25e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.34e-01

Confidence level: 3.24e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Naphthylamine</div> <div>Measured: 4.00e-01</div> <div>Predicted: 9.37e-04</div>	<div>Image not found</div> <div>2-Butanone, 1-bromo-</div> <div>Measured: 1.26e-01</div> <div>Predicted: 7.89</div>	<div>Image not found</div> <div>Nonylamine</div> <div>Measured: 1.55e-01</div> <div>Predicted: 2.75e-01</div>
<div>Image not found</div> <div>Piperophos</div> <div>Measured: 5.48e-02</div> <div>Predicted: 3.95e-07</div>	<div>Image not found</div> <div>Benazolin-ethyl</div> <div>Measured: 2.89e-07</div> <div>Predicted: 9.58e-07</div>	